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A surrogate-assisted evolutionary algorithm based on the genetic diversity objective

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ABSTRACT

In this work, a novel surrogate-assisted memetic algorithm is proposed which is based on the preservation of genetic diversity within the population. The aim of the algorithm is to solve multi-objective optimization problems featuring computationally expensive fitness functions in an efficient manner. The main novelty is the use of an evolutionary algorithm as global searcher that treats the genetic diversity as an objective during the evolution and uses it, together with a non-dominated sorting approach, to assign the ranks. This algorithm, coupled with a gradient-based algorithm as local searcher and a back-propagation neural network as global surrogate model, demonstrates to provide a reliable and effective balance between exploration and exploitation. A detailed performance analysis has been conducted on five commonly used multi-objective problems, each one involving distinct features that can make the convergence difficult toward the Pareto-optimal front. In most cases, the proposed algorithm outperformed the other state-of-the-art evolutionary algorithms considered in the comparison, assuring higher repeatability on the final non-dominated set, deeper convergence level and higher convergence rate. It also demonstrates a clear ability to widely cover the Pareto-optimal front with larger percentage of non-dominated solutions if compared to the total number of function evaluations.

1. Introduction

In recent years, the research toward building advanced multi-objective evolutionary algorithms (MOEAs) for solving complex problems involving multiple conflicting objectives have been increasing enormously [1]. In particular, the need for effective optimization tools dealing with computationally expensive objective functions and constraints has become widespread in almost all the engineering disciplines. One of these is computational fluid dynamics (CFD), a set of numerical techniques which makes it possible to solve for the Reynolds-averaged Navier–Stokes (RANS) equations in complex domains, where a single run can require a huge computational effort.

In those cases, the modeling and design optimization cycle time is roughly proportional to the number of calls to the computationally expensive solver, so that many evolutionary frameworks have been implemented around the idea of alleviating the computational cost by introducing an approximate, or surrogate, model of the real objective functions [2,3]. The surrogate model (SM) is actually a model of the mathematical model itself upon which the solver is built, and therefore con be referred to as a "metamodel".

Using a SM has become a very popular approach since the efforts required to build the surrogates and to use them along with MOEAs are much lower than those in the standard, direct-call methodologies [4]. Popular SM are built using several methodologies, e.g. parametric statistical methods such as the response surface methodology (RSM) [5–7] as well as nonparametric techniques [8–10], like multivariate adaptive regression splines [11], artificial neural networks (ANNs) [12] and radial basis functions (RBFs) [13–15]. Other, more recently developed, nonparametric techniques for surrogate modeling encompass support vector regression (SVR) [16–18], regression Kriging (RK) [19–22] and moving least squares or local polynomial regression (LPR) [23–27].

In the framework of MOEAs, several approaches for dealing with computationally expensive problems using surrogate models have been documented in the open literature. First approaches were based on the concept of fitness inheritance [28,29], where the fitness of an individual is evaluated indirectly by interpolating the fitness of its parents. Evolution control techniques, e.g. clustering methods [30,31], were also proposed as a way to estimate when exact function evaluations are to be performed.

Alternative approaches utilize a progressive refinement of a SM as the search evolves [32]. Within those methodologies, memetic

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algorithms (MAs) seem to be one of the most promising techniques [33].

MAs are population-based metaheuristic search methods that follow the basis of Dawkins notion of "meme", defined as a unit of cultural evolution that is capable of local refinements [34–36]. MAs have also been used under the name of hybrid evolutionary algorithms, Baldwinian evolutionary algorithms, Lamarkian evolutionary algorithms, or genetic local search [33]. The main advantage of MAs over concurrent strategies lies in creating a synergy between global and local search of a set of optimal solutions of the objective function. A SM can be used in lieu of the original, computationally expensive, objective function during the local refinement thus leading to the so-called surrogate-assisted memetic algorithm (SAMA) concept. To this purpose, the prediction accuracy of fitness predictions based on SMs can be significantly enhanced with the inclusion of gradient information in SM building [37,38].

It has been extensively demonstrated in literature [39–41] that diversity preservation during evolution is a crucial aspect for evolutionary algorithms (EAs). If the lack of population diversity occurs too early the algorithm is trapped in confined regions and is not able to explore the whole search space. The diversity preservation becomes particularly important in the case of MAs [42,43] and SAMAs because of their marked tendency to exploitation. In this paper, a novel multi-objective SAMA is introduced and described which is based on the coupling between the genetic diversity evolutionary algorithm (GeDEA) [39] as global searcher and a local search framework built around a gradient-based algorithm working with a SM of the original optimization function. Because of its peculiar features we named it the genetic diversity memetic algorithm (GDMA).

In the following chapters the rationale behind the development of the proposed algorithm is presented, starting with a brief recall about the importance of preserving diversity during evolution for genetic and memetic algorithms. The main methodologies used in literature to face such a problem are listed and compared with the selected diversity preservation method [39]. Second the GDMA is presented together with the metamodeling technique used to build the local search framework, and the framework itself. In the final stage GDMA is applied to five, commonly used, test functions in order to compare its performance against several well-known evolutionary algorithms by means of four different performance metrics. GDMA is then used on a real-world application where a multi-objective/multi-point optimization of a 2D aerodynamic airfoil is carried out.

2. The preservation of genetic diversity

The genetic diversity of individuals for population-based algorithms has been recognized as a crucial property since the beginning of the subject [44] and many works were conducted with the aim of improving the performance of an algorithm by introducing specific diversity preservation strategies. As already mentioned the selective pressure driving toward optimal solutions can lead to a rapid impoverishment of the genetic material within the population, with consequent premature convergence of the algorithm. The strategies used in literature to prevent such a circumstance in GAs are many, in the following we briefly recall and describe the most relevant ones:

- Crowding: it consists on the replacement of existing individuals on the parent population that present similarities on a genotypic viewpoint. The strategies differ for the way they select and replace the most similar elements inside the population. Deterministic [40,45] and probabilistic [46] crowding methods have been used. Other crowding algorithms are Metropolis algorithm [47], restricted tournament selection [48] and simulated annealing [49], which can be all considered local tournament algorithms [50].
- Niching: these techniques consist on promoting the formation within the population of stable sub-populations (niches) [51] which contain different genetic information. They are traditionally used in domains when the finding of multiple solutions is desired, such as in optimization of multi-modal functions. The most frequently used niching technique is the fitness sharing [52].
- Diversity as an objective: the idea of using the diversity as an objective during the evolution was first in [39]. The diversity, measured in terms of the Euclidean distance from the other individuals, is used in the ranking procedure thanks to a non-dominated sorting of (i) the diversity and (ii) the ranks scored with respect to the objectives of the original MOOP. In [53,54] instead the diversity is used as an additional objective, increasing the dimensionality of the original MOOP.
- Other methods: additional methods are available in literature like multiploidy [55], DCGA (diversity control oriented GA) [56], CSGA (complementary surrogate GA) [57], TMPGA (Tabu multi parent GA) [58], FUSS (fitness uniform selection scheme) [59] and other strategies not cited here.

The importance of diversity has been highlighted also in some works where basic MAs (without the use of SMs) were used. In [60,61] the diversity has been used during the evolution of a parallel memetic algorithm (PMA) in order to dynamically control the local search frequency with the aim of reducing the number of function evaluations. On a similar fashion the individuals' diversity has been considered in [62] with the only difference that here it is used to decide between three different local searchers of an adaptive MA. The works considered so far treat the diversity as an indirect parameter to adapt the local search strategy, which is not strictly a diversity preservation technique. On the contrary in [63] a MA is improved by direct population management removing solutions that are below a certain threshold in terms of distance from the other individuals. Again in [42] the population diversity is preserved in a bacterial MA by means of hibernation of individuals. The idea is to hibernate some bacteria for a while. Then the hibernated bacteria can help in directing back the evolutionary process to right way if it convergences to local optima. No works are known at the moment of writing about diversity preservation techniques implemented in SAMAs.

In previous paragraph we stated the significance of preserving diversity within the evolutionary process in EAs and this is confirmed by the great importance that this subject has had in literature and the large number of works done on it. Diversity is considered as an important factor for classic GAs but it becomes crucial for MAs and SAMAs. These types of algorithms are specifically designed to emphasize the selective pressure mechanism toward the Pareto optimal set, thanks to the local search framework embedded. For this reason they are much more subject to premature convergence and impoverishment of the genotypic diversity within the population and a diversity preservation strategy is mandatory.

3. The genetic diversity memetic algorithm (GDMA)

The proposed optimization strategy consists in a SAMA strategy which is based on the genetic diversity preservation method GeDEA [39]. The GeDEA is here used as global searcher while additional tools are selected in order to set up a SAMA methodology. An ANN is selected as objective function's surrogate model and a Local Search Framework is built to perform local refinements of the